

EFFECT OF EXTERNAL MAGNETIC FIELD ON THE CO-EXISTENCE OF SUPERCONDUCTIVITY AND ANTIFERROMAGNETISM IN RARE EARTH NICKEL BOROCARBIDES (RNi_2B_2C)

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Abstract

In this paper we have studied the effect of external magnetic field in the co-existing phase of superconducting and anti-ferromagnetism of rare earth nickel borocarbides. The anti-ferromagnetism in these systems might have originated due to both localized 'f' electrons as well as itinerant electrons which are responsible for conduction. On the other hand, superconductivity is due to spin density wave, arising out of Fermi surface instability. The anti-ferromagnetism order is mostly influenced by hybridization of the 'f' electron with the conduction electron. Here we have obtained the dependence of superconducting energy gap as well as staggered magnetic field on temperature T and energy ϵ_k in a framework based on mean field Hamiltonian using double time electron Green's function. We have shown in our calculation the effect of external magnetic field on superconducting and anti-ferromagnetic order parameter for YNi_2B_2C in the presence of hybridization. The ratio of the calculated effective gap and T_C is close to BCS value which agrees quite well with experimental results.

1 Introduction

The rare earth nickel borocarbide RNi_2B_2C ($R = Y, Lu, Tm, Er, Ho, Dy$) compounds are known for exhibiting both superconductivity and long range anti-ferromagnetic order[1-2]. These compounds have two generally conflicting long range orders in an accessible temperature range and thus have attracted the attention of many researchers in this field[1-4]. They have layer structure consisting of $R - C$ sheets separated by Ni_2B_2 layers along the crystallographic c-axis[3] similar to that of high T_c superconductors. In spite of the layered structure these compounds have isotropic normal state which are supported by band structure calculation[5,6]. This result is supported experimentally by calculated resistivity data in single crystal YNi_2B_2C [7]. An explicit study on these compounds can disclose many effects on the relationship between superconductivity and anti-ferromagnetism[8-9]. Hence, the large electron-electron coupling, high phonon frequencies and considerably large density of states at the Fermi surface, give evidence of the phonon mediated BCS mechanism for superconductivity[6,9,10]. The experimental data shows an anisotropic[3] nature of the superconducting state, which contradict with other observed data. In upper critical field measurement, $LuNi_2B_2C$ exhibits anisotropy when magnetic field is applied parallel and perpendicular to c-axis which is not shown by Y- compounds[3,11]. Similarly, the experimental data on thermal conductivity[12] and photo-emission spectroscopic measurement [13] show large anisotropy[14] with the existence of node in the superconducting gap function. The specific heat, magnetization and resistivity measurements point towards the s-wave symmetry and the pairing is mediated by the electron-phonon interaction[15].

From the band structure calculation[5,6] of borocarbides, it is found that one of the four bands crossing the Fermi level is a flat one indicates the system being a correlated one. This flat band has the largest contribution to the density of states at Fermi surface suggesting it's dominance in the formation of superconducting state [6,16]. On the other hand, the flat band hybridizes with the conduction band formed out of other three bands (consisting of Y, B, C). There is a peak in the density of states at the Fermi level to which the d-band of nickel and bands of Y(5d),B(2p)and C(2p) electrons [5,6,16] contribute. Here we have extended the model as proposed by Fulde and others[17-20] to study the co-existence of superconductivity (SC) and anti-ferromagnetism (AFM) in presence of external magnetic field. In the present communication, we have included hybridization effect and the study of the effect of external magnetic field on the order parameters. The organization of the paper reflects: In section 2, the framework of our model is briefly presented, where we have obtained the equation for superconducting and staggered magnetic field gap parameter by using double time Green function of Zubarev type[21]. Section 3 explains

parameters for numerical calculation and discussion. Finally section 4 provides the concluding remark.

2 Theoretical Framework

Superconductivity in the rare-earth nickel borocarbides can be described by the usual BCS theory mediated by the phonon. The anti-ferromagnet might have originated from both the localized f-electrons and itinerant electrons responsible for conduction. The itinerant electron which arises from spin density wave (SDW) due to Fermi surface instability contributed to AFM, is also responsible for superconductivity. Thus the localized magnetic moments due to staggered sub lattice magnetization co-exists with superconductivity. Besides this, the electrons in a localized level hybridize with the conduction electrons near the Fermi level. Fulde et al [17] while describing the heavy fermion behaviour for copper oxide superconductors, showed that the f-level of the rare earth atoms hybridizes with the conduction band. In case of rare earth nickel borocarbides, the f-level of the rare earth atoms lies too far below the Fermi level to affect the electronic properties of the system as seen from band structure calculations [5,6]. Due to hybridization, the sub-lattice AFM acquire the character of localized state of the flat d-band[18]. The order parameters corresponding to the AFM and the SC long range orders have been calculated for rare earth nickel borocarbides[18,19]. In our model Hamiltonian present below, we have included the effect of hybridization in presence of external magnetic field. The anti-ferromagnetic exchange leads to long range anti ferromagnetic order due to the spin alignment in Ni lattice site. This helps in dividing Ni lattice into two sub-lattices. If A and B denote two sub-lattice of Ni system, the Hamiltonian expressed in [17,18] can be extended to

$$\begin{aligned}
H = & \sum_{\mathbf{k}, \sigma} \epsilon_o(\mathbf{k}) (a_{\mathbf{k}\sigma}^\dagger b_{\mathbf{k}\sigma} + h.c.) + \left(\frac{\hbar}{2}\right) \sum_{\mathbf{k}\sigma} \sigma (a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma} - b_{\mathbf{k}\sigma}^\dagger b_{\mathbf{k}\sigma}) \\
& + V \sum_{\mathbf{k}\sigma} (a_{\mathbf{k}\sigma}^\dagger f_{1,\mathbf{k}\sigma} + b_{\mathbf{k}\sigma}^\dagger f_{2,\mathbf{k}\sigma} + h.c.) - \Delta \sum_{\mathbf{k}} \left[(a_{\mathbf{k}\uparrow}^\dagger a_{-\mathbf{k}\downarrow}^\dagger + h.c.) + (b_{\mathbf{k}\uparrow}^\dagger b_{-\mathbf{k}\downarrow}^\dagger + h.c.) \right] \\
& + \sum_{\mathbf{k}\sigma} (\epsilon_f + \sigma g \mu_B B) \sum_{\mathbf{k}\sigma, i=1,2} f_{i\mathbf{k}\sigma}^\dagger f_{i\mathbf{k}\sigma} + g \mu_B B \sum_{\mathbf{k}\sigma} \sigma (a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma} + b_{\mathbf{k}\sigma}^\dagger b_{\mathbf{k}\sigma}) \quad (1)
\end{aligned}$$

where \mathbf{k} , σ $a_{\mathbf{k}\sigma}^\dagger$ ($a_{\mathbf{k}\sigma}$) and $b_{\mathbf{k}\sigma}^\dagger$ ($b_{\mathbf{k}\sigma}$) are the momentum, spin, creation (annihilation) operators of electrons belonging to the two sub lattices A and B respectively. The first term describes the hopping of conduction electrons between neighbouring sites of Ni and dispersion[17] is given by

$$\epsilon_o(\mathbf{k}) = -2t(\cos k_x + \cos k_y) \quad (2)$$

here t is the nearest neighbour hopping integral. The lattice constant has been set equal to unity. The second term is due to staggered magnetic field h arising from Heisenberg exchange interaction between the magnetic moments of neighboring sites. This field acts on the Ni spins and strongly reduces the charge fluctuation between different sites [18]. 'h' is the strength of the sub lattice magnetisation (also anti-ferromagnetic order parameter) and is expressed [18] as

$$h = -\frac{1}{2}g\mu_B \sum_{\mathbf{k}\sigma} \left[\langle a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma} \rangle - \langle b_{\mathbf{k}\sigma}^\dagger b_{\mathbf{k}\sigma} \rangle \right] \quad (3)$$

g and μ_B being the Lande g factor and Bohr magneton, respectively. The third term describes the effective hybridization. V is the hybridization interaction constant [17] and is taken to be independent of \mathbf{k} . For simplicity we have taken on-site hybridization (the localized electron belonging to sub-lattice 1 hybridize with the conduction electron of that sub-lattice alone and so on). The fourth term describes the attractive interaction of the charge carriers on the Ni_2B_2 planes leading to cooper pair formation. We have considered BCS type phonon mediated cooper pairing for superconductivity and intra sub-lattice cooper pairing is assumed to make the calculation simpler. The superconducting gap parameter (Δ) is defined as

$$\Delta = - \sum_k \tilde{V}_k \left(\langle a_{k\uparrow}^\dagger a_{-k\downarrow}^\dagger \rangle + \langle b_{k\uparrow}^\dagger b_{-k\downarrow}^\dagger \rangle \right) \quad (4)$$

\tilde{V}_k is the strength of the attractive interaction between two electrons mediated by phonon. The intra f-electron Hamiltonian in presence of magnetic field is given by

$$H_f = (\epsilon_f + \frac{1}{2}g\mu_B B) \sum_{\mathbf{i}, \mathbf{k}_i=1,2} f_{ik\uparrow}^\dagger f_{ik\uparrow} + (\epsilon_f - \frac{1}{2}g\mu_B B) \sum_{\mathbf{i}, \mathbf{k}_i=1,2} f_{ik\downarrow}^\dagger f_{ik\downarrow} \quad (5)$$

ϵ_f is the dispersion less re normalized f-level energy of the rare earth ions. $f_{ik\sigma}^\dagger$ ($f_{ik\sigma}$) is the creation (annihilation) operator of the localized electron in the two sub-lattices ($i=1,2$). The external magnetic field acts on moments of rare earth and Ni element which are parallel to each other. As a result, the external field splits the two field degenerate bands and new quasi particle energies are obtained. ($\epsilon_F \rightarrow \epsilon_F \pm \frac{1}{2}g\mu_B B$). The Hamiltonian due to external magnetic field B on the Ni lattice is given by

$$H_B = \frac{1}{2}g\mu_B B \left[\sum_{\vec{k}} (a_{\vec{k}\uparrow}^\dagger a_{\vec{k}\uparrow} + b_{\vec{k}\uparrow}^\dagger b_{\vec{k}\uparrow}) - \sum_{\vec{k}} (a_{\vec{k}\downarrow}^\dagger a_{\vec{k}\downarrow} + b_{\vec{k}\downarrow}^\dagger b_{\vec{k}\downarrow}) \right] \quad (6)$$

2.1 Superconducting gap

We study the Hamiltonian given in equation (1) with the help of Green's function technique using the equation of motion for the single particle green function of Zubarev type [21]. We have defined the green functions $A_i(k, w)$, $B_i(k, w)$, $C_i(k, w)$, $D_i(k, w)$ ($i=1,6$). We have considered the following Green functions in our present calculation.

$$\begin{aligned}
A_1(\mathbf{k}, \omega) &= \ll a_{\mathbf{k}\uparrow}; a_{\mathbf{k}\uparrow}^\dagger \gg_\omega \\
A_2(\mathbf{k}, \omega) &= \ll a_{-\mathbf{k}\downarrow}^\dagger; a_{\mathbf{k}\uparrow}^\dagger \gg_\omega \\
B_1(\mathbf{k}, \omega) &= \ll b_{\mathbf{k}\uparrow}; b_{\mathbf{k}\uparrow}^\dagger \gg_\omega \\
B_2(\mathbf{k}, \omega) &= \ll b_{-\mathbf{k}\downarrow}^\dagger; b_{\mathbf{k}\uparrow}^\dagger \gg_\omega \\
C_1(\mathbf{k}, \omega) &= \ll a_{\mathbf{k}\downarrow}; a_{\mathbf{k}\downarrow}^\dagger \gg_\omega \\
D_1(\mathbf{k}, \omega) &= \ll b_{\mathbf{k}\downarrow}; b_{\mathbf{k}\downarrow}^\dagger \gg_\omega
\end{aligned} \tag{7}$$

For our convenience, we have dropped the \mathbf{k} and w dependence of Green's function. The Fermi level is taken as zero ($\epsilon_F = 0$) and the re-normalized localized f energy level is assumed to coincide with the Fermi level for simplicity. The above Green's functions are evaluated by using equation of motion and commutation relation of the fermion operators $a_{k\sigma}$, $b_{k\sigma}$, $f_{1k\sigma}$. The coupled equations in $A_i(k, \omega)$, $B_i(k, \omega)$, $C_i(k, \omega)$, $D_i(k, \omega)$ for $i = 1, 2$ are solved and those equations can be expressed in form of

$$A_{1,2} = \frac{\omega'}{4\pi} \left[\frac{\omega'(\omega' - (\Delta - \frac{h}{2})) - V^2}{\omega'^4 - \omega'^2 E_{1k}^2 + V^4} \pm \frac{\omega'(\omega' + (\Delta + \frac{h}{2})) - V^2}{\omega'^4 - \omega'^2 E_{2k}^2 + V^4} \right] \tag{8}$$

$$B_{1,2} = \frac{\omega'}{4\pi} \left[\frac{\omega'(\omega' - (\Delta + \frac{h}{2})) - V^2}{\omega'^4 - \omega'^2 E_{2k}^2 + V^4} \pm \frac{\omega'(\omega' + (\Delta - \frac{h}{2})) - V^2}{\omega'^4 - \omega'^2 E_{1k}^2 + V^4} \right] \tag{9}$$

$$C_1 = \frac{\omega''}{4\pi} \left[\frac{\omega''(\omega'' + (\Delta - \frac{h}{2})) - V^2}{\omega''^4 - \omega''^2 E_{1k}^2 + V^4} + \frac{\omega''(\omega'' - (\Delta + \frac{h}{2})) - V^2}{\omega''^4 - \omega''^2 E_{2k}^2 + V^4} \right] \tag{10}$$

$$D_1 = \frac{\omega''}{4\pi} \left[\frac{\omega''(\omega'' + (\Delta + \frac{h}{2})) - V^2}{\omega''^4 - \omega''^2 E_{2k}^2 + V^4} + \frac{\omega''(\omega'' - (\Delta - \frac{h}{2})) - V^2}{\omega''^4 - \omega''^2 E_{1k}^2 + V^4} \right] \tag{11}$$

where

$$\begin{aligned}
E_{1k}^2 &= \epsilon_{1k}^2 + 2V^2 \\
E_{2k}^2 &= \epsilon_{2k}^2 + 2V^2 \\
\epsilon_{1k}^2 &= \epsilon_0^2(k) + \left(\Delta - \frac{h}{2}\right)^2 \\
\epsilon_{2k}^2 &= \epsilon_0^2(k) + \left(\Delta + \frac{h}{2}\right)^2
\end{aligned} \tag{12}$$

and

$$\begin{aligned}
\omega' &= \omega - \frac{1}{2}g\mu_B B \\
h' &= h + g\mu_B B \\
h'' &= h - g\mu_B B
\end{aligned} \tag{13}$$

In the limit, when $h \rightarrow 0$, equation (12) reduces to BCS expression. The two band vanishes in the absence of hybridization. The existence of four distinct bands in presence of hybridization indicates the co-existence of anti-ferromagnetism and superconductivity. In the limiting condition when $\frac{h}{2} \rightarrow \Delta$, $\epsilon_{1k} \rightarrow \pm\epsilon_0(k)$, superconductivity is suppressed by the anti-ferromagnetism. Similarly $\epsilon_{2k} \rightarrow \pm[\epsilon_0^2(k) + 2\Delta^2]^{\frac{1}{2}}$ shows superconductivity is enhanced by the anti-ferromagnetic order in these two bands. The poles of the Green's functions $A_{1,2}(w), B_{1,2}(w), C_1(w), D_1(w)$ are obtained from

$$\begin{aligned}
\omega'^4 - \omega'^2 E_{1k}^2 + V^4 &= 0 \\
\omega'^4 - \omega'^2 E_{2k}^2 + V^4 &= 0
\end{aligned} \tag{14}$$

The solutions of the above equations are eight poles of the Green's functions $A_{1,2}(k, \omega), B_{1,2}(k, \omega)$. Solving the equation (14), we get

$$\begin{aligned}
\omega'_{1\pm} &= \pm \sqrt{\frac{1}{2}(E_{1k}^2 + \sqrt{E_{1k}^4 - 4V^4})} \\
\omega'_{2\pm} &= \pm \sqrt{\frac{1}{2}(E_{2k}^2 - \sqrt{E_{2k}^4 - 4V^4})}
\end{aligned} \tag{15}$$

and

$$\begin{aligned}\omega'_{3\pm} &= \pm \sqrt{\frac{1}{2}(E_{2k}^2 + \sqrt{E_{2k}^4 - 4V^4})} \\ \omega'_{4\pm} &= \pm \sqrt{\frac{1}{2}(E_{2k}^2 - \sqrt{E_{2k}^4 - 4V^4})}\end{aligned}\quad (16)$$

These eight poles give eight quasi particle energy bands $\omega'_{i\pm}$ ($i = 1$ to 4). The superconducting gap parameter (Δ) in equation (4) can be explicitly written in terms of temperature dependent parameter and its integral form which can be expressed as

$$\Delta(T) = -\sum_k \tilde{V}_k \left[\langle a_{\mathbf{k}\uparrow}^\dagger a_{-\mathbf{k}\downarrow}^\dagger \rangle + \langle b_{\mathbf{k}\uparrow}^\dagger b_{-\mathbf{k}\downarrow}^\dagger \rangle \right] \quad (17)$$

and

$$\Delta(T) = -\tilde{V} N(0) \int_{-\omega_D}^{+\omega_D} d\epsilon_0(\mathbf{k}) \left[\langle a_{\mathbf{k}\uparrow}^\dagger a_{-\mathbf{k}\downarrow}^\dagger \rangle + \langle b_{\mathbf{k}\uparrow}^\dagger b_{-\mathbf{k}\downarrow}^\dagger \rangle \right] \quad (18)$$

$N(0)$ is the density of state of the conduction electrons at the Fermi level ϵ_F and ω_D is the Debye frequency. The limitation on the \mathbf{k} sum is due to the restriction of attractive interaction, which is effective with energies $|\epsilon_1 - \epsilon_2| < \omega_D$. In the weak coupling limit, the interaction potential \tilde{V}_k is

$$\begin{aligned}\tilde{V}_k &= -V_0 & \text{if } |\epsilon_1 - \epsilon_2| < \omega_D \\ &= 0 & \text{otherwise}\end{aligned}$$

Approximating the gap parameter to be independent of \mathbf{k} , We can derive the equations for single particle co-relation function as [17,18]

$$\langle a_{\mathbf{k}\uparrow}^\dagger a_{-\mathbf{k}\downarrow}^\dagger \rangle + \langle b_{\mathbf{k}\uparrow}^\dagger b_{-\mathbf{k}\downarrow}^\dagger \rangle = i \lim_{\epsilon \rightarrow 0} \int \frac{d\omega}{(e^{\beta\omega} + 1)} [A_2 B_2(\omega + i\epsilon) - A_2 B_2(\omega - i\epsilon)] \quad (19)$$

Using equations (8) and (9) in equation (19), we obtain as

$$\begin{aligned}
\langle a_{\vec{k}\uparrow}^\dagger a_{-\vec{k}\downarrow}^\dagger \rangle + \langle b_{\vec{k}\uparrow}^\dagger b_{-\vec{k}\downarrow}^\dagger \rangle = & \left[\frac{\Delta - \frac{\hbar}{2}}{2\sqrt{E_{1k}^4 - 4V^4}} \left\{ \omega'_1 \left(\frac{1}{e^{\beta\frac{\alpha}{2}} e^{\beta\omega'_1} + 1} - \frac{1}{e^{\beta\frac{\alpha}{2}} e^{-\beta\omega'_1} + 1} \right) \right. \right. \\
& \left. \left. - \omega'_2 \left(\frac{1}{e^{\beta\frac{\alpha}{2}} e^{\beta\omega'_2} + 1} - \frac{1}{e^{\beta\frac{\alpha}{2}} e^{-\beta\omega'_2} + 1} \right) \right\} \right. \\
& + \frac{\Delta + \frac{\hbar}{2}}{2\sqrt{E_{2k}^4 - 4V^4}} \left\{ \omega'_3 \left(\frac{1}{e^{\beta\frac{\alpha}{2}} e^{\beta\omega'_3} + 1} - \frac{1}{e^{\beta\frac{\alpha}{2}} e^{-\beta\omega'_3} + 1} \right) \right. \\
& \left. \left. - \omega'_4 \left(\frac{1}{e^{\beta\frac{\alpha}{2}} e^{\beta\omega'_4} + 1} - \frac{1}{e^{\beta\frac{\alpha}{2}} e^{-\beta\omega'_4} + 1} \right) \right\} \right] \quad (20)
\end{aligned}$$

The expression for the superconducting order parameter can be restructured as

$$\Delta(T) = -\tilde{V}N(0) \int_{-w_D}^{+w_D} d\epsilon_o(k) [F_1(\vec{k}, T) + F_2(\vec{k}, T)] \quad (21)$$

where

$$\begin{aligned}
F_1(\vec{k}, T) = & \frac{\Delta - \frac{\hbar}{2}}{2\sqrt{E_{1k}^4 - 4V^4}} \left\{ \omega'_1 \left(\frac{1}{e^{\beta\frac{\alpha}{2}} e^{\beta\omega'_1} + 1} - \frac{1}{e^{\beta\frac{\alpha}{2}} e^{-\beta\omega'_1} + 1} \right) \right. \\
& \left. - \omega'_2 \left(\frac{1}{e^{\beta\frac{\alpha}{2}} e^{\beta\omega'_2} + 1} - \frac{1}{e^{\beta\frac{\alpha}{2}} e^{-\beta\omega'_2} + 1} \right) \right\} \quad (22)
\end{aligned}$$

and

$$\begin{aligned}
F_2(\vec{k}, T) = & \frac{\Delta + \frac{\hbar}{2}}{2\sqrt{E_{2k}^4 - 4V^4}} \left\{ \omega'_3 \left(\frac{1}{e^{\beta\frac{\alpha}{2}} e^{\beta\omega'_3} + 1} - \frac{1}{e^{\beta\frac{\alpha}{2}} e^{-\beta\omega'_3} + 1} \right) \right. \\
& \left. - \omega'_4 \left(\frac{1}{e^{\beta\frac{\alpha}{2}} e^{\beta\omega'_4} + 1} - \frac{1}{e^{\beta\frac{\alpha}{2}} e^{-\beta\omega'_4} + 1} \right) \right\} \quad (23)
\end{aligned}$$

2.2 Staggered Magnetic Field h

The staggered magnetic field h as given in equation (3) is responsible for anti-ferromagnetism and is assumed to be constant. The expression for staggered magnetic field strength in presence of external magnetic field is given as

$$h = -\frac{1}{2}g\mu_B \sum_{\mathbf{k}} [\{ \langle a_{\mathbf{k}\uparrow}^\dagger a_{\mathbf{k}\uparrow} \rangle - \langle b_{\mathbf{k}\uparrow}^\dagger b_{\mathbf{k}\uparrow} \rangle \} - \{ \langle a_{\mathbf{k}\downarrow}^\dagger a_{\mathbf{k}\downarrow} \rangle - \langle b_{\mathbf{k}\downarrow}^\dagger b_{\mathbf{k}\downarrow} \rangle \}] \quad (24)$$

and

$$h = -\frac{N(0)}{2}g\mu_B \int_{+\frac{w}{2}}^{-\frac{w}{2}} d\epsilon_0(k) \left[\left\{ \langle a_{\mathbf{k}\uparrow}^\dagger a_{\mathbf{k}\uparrow} \rangle - \langle b_{\mathbf{k}\uparrow}^\dagger b_{\mathbf{k}\uparrow} \rangle \right\} - \left\{ \langle a_{\mathbf{k}\downarrow}^\dagger a_{\mathbf{k}\downarrow} \rangle - \langle b_{\mathbf{k}\downarrow}^\dagger b_{\mathbf{k}\downarrow} \rangle \right\} \right] \quad (25)$$

Calculating the co-relation function $\langle a_{\mathbf{k}\uparrow}^\dagger a_{\mathbf{k}\uparrow} \rangle$, $\langle a_{\mathbf{k}\downarrow}^\dagger a_{\mathbf{k}\downarrow} \rangle$, $\langle b_{\mathbf{k}\uparrow}^\dagger b_{\mathbf{k}\uparrow} \rangle$ and $\langle b_{\mathbf{k}\downarrow}^\dagger b_{\mathbf{k}\downarrow} \rangle$ from the Green's functions $A_1(\mathbf{k}, \omega)$, $B_1(\mathbf{k}, \omega)$, $C_1(\mathbf{k}, \omega)$, and $D_1(\mathbf{k}, \omega)$, respectively, we can express the staggered magnetic field 'h' as

$$h = -\frac{1}{2}g\mu_B \sum_{\vec{k}} \left[\left\{ i \lim_{\epsilon \rightarrow 0} \int \frac{d\omega}{e^{\beta\omega} + 1} (A_1 B_1(\omega + i\epsilon) - A_1 B_1(\omega - i\epsilon)) \right\} - \left\{ i \lim_{\epsilon \rightarrow 0} \int \frac{d\omega}{e^{\beta\omega} + 1} (C_1 D_1(\omega + i\epsilon) - C_1 D_1(\omega - i\epsilon)) \right\} \right] \quad (26)$$

$$A_1 B_1(\omega) = \ll a_{\vec{k}\uparrow}^\dagger a_{\vec{k}\uparrow} \gg - \ll b_{\vec{k}\uparrow}^\dagger b_{\vec{k}\uparrow} \gg = A_1(\omega) - B_1(\omega) \quad (27)$$

and

$$C_1 D_1(\omega) = \ll a_{\vec{k}\downarrow}^\dagger a_{\vec{k}\downarrow} \gg - \ll b_{\vec{k}\downarrow}^\dagger b_{\vec{k}\downarrow} \gg = C_1(\omega) - D_1(\omega) \quad (28)$$

Solving the above equations we can represent as

$$A_1(\omega) - B_1(\omega) = - \left[\frac{\Delta - \frac{\hbar}{2}}{2\sqrt{E_{1k}^4 - 4V^4}} \left\{ \omega'_1 \left(\frac{1}{e^{\beta\frac{\alpha}{2}} e^{\beta\omega'_1} + 1} - \frac{1}{e^{\beta\frac{\alpha}{2}} e^{-\beta\omega'_1} + 1} \right) - \omega'_2 \left(\frac{1}{e^{\beta\frac{\alpha}{2}} e^{\beta\omega'_2} + 1} - \frac{1}{e^{\beta\frac{\alpha}{2}} e^{-\beta\omega'_2} + 1} \right) \right\} + \frac{\Delta + \frac{\hbar}{2}}{2\sqrt{E_{2k}^4 - 4V^4}} \left\{ \omega'_3 \left(\frac{1}{e^{\beta\frac{\alpha}{2}} e^{\beta\omega'_3} + 1} - \frac{1}{e^{\beta\frac{\alpha}{2}} e^{-\beta\omega'_3} + 1} \right) - \omega'_4 \left(\frac{1}{e^{\beta\frac{\alpha}{2}} e^{\beta\omega'_4} + 1} - \frac{1}{e^{\beta\frac{\alpha}{2}} e^{-\beta\omega'_4} + 1} \right) \right\} \right] \quad (29)$$

and

$$\begin{aligned}
C_1(\omega) - D_1(\omega) = & \left[\frac{\Delta - \frac{\hbar}{2}}{2\sqrt{E_{1k}^4 - 4V^4}} \left\{ \omega_1'' \left(\frac{1}{e^{-\beta\frac{\alpha}{2}} e^{\beta\omega_1''} + 1} - \frac{1}{e^{-\beta\frac{\alpha}{2}} e^{-\beta\omega_1''} + 1} \right) \right. \right. \\
& \left. \left. - \omega_2'' \left(\frac{1}{e^{-\beta\frac{\alpha}{2}} e^{\beta\omega_2''} + 1} - \frac{1}{e^{-\beta\frac{\alpha}{2}} e^{-\beta\omega_2''} + 1} \right) \right\} \right. \\
& \left. - \frac{\Delta + \frac{\hbar}{2}}{2\sqrt{E_{1k}^4 - 4V^4}} \left\{ \omega_3'' \left(\frac{1}{e^{-\beta\frac{\alpha}{2}} e^{\beta\omega_3''} + 1} - \frac{1}{e^{-\beta\frac{\alpha}{2}} e^{-\beta\omega_3''} + 1} \right) \right. \right. \\
& \left. \left. - \omega_4'' \left(\frac{1}{e^{-\beta\frac{\alpha}{2}} e^{\beta\omega_4''} + 1} - \frac{1}{e^{-\beta\frac{\alpha}{2}} e^{-\beta\omega_4''} + 1} \right) \right\} \right] \quad (30)
\end{aligned}$$

where

$$i \lim_{\epsilon \rightarrow 0} \int \frac{d\omega}{e^{\beta\omega} + 1} [A_1 B_1(\omega + i\epsilon) - A_1 B_1(\omega - i\epsilon)] = - \left[F_1(\vec{k}, T) - F_2(\vec{k}, T) \right] \quad (31)$$

and

$$i \lim_{\epsilon \rightarrow 0} \int \frac{d\omega}{e^{\beta\omega} + 1} [C_1 D_1(\omega + i\epsilon) - C_1 D_1(\omega - i\epsilon)] = \left[F_3(\vec{k}, T) - F_4(\vec{k}, T) \right] \quad (32)$$

The extra term F_3 and F_4 are obtained due to application of magnetic field in presence of hybridization. Where

$$\begin{aligned}
F_3(\vec{k}, T) = & \frac{\Delta - \frac{\hbar}{2}}{2\sqrt{E_{1k}^4 - 4V^4}} \left\{ \omega_1'' \left(\frac{1}{e^{-\beta\frac{\alpha}{2}} e^{\beta\omega_1''} + 1} - \frac{1}{e^{-\beta\frac{\alpha}{2}} e^{-\beta\omega_1''} + 1} \right) \right. \\
& \left. - \omega_2'' \left(\frac{1}{e^{-\beta\frac{\alpha}{2}} e^{\beta\omega_2''} + 1} - \frac{1}{e^{-\beta\frac{\alpha}{2}} e^{-\beta\omega_2''} + 1} \right) \right\} \quad (33)
\end{aligned}$$

and

$$\begin{aligned}
F_4(\vec{k}, T) = & \frac{\Delta + \frac{\hbar}{2}}{2\sqrt{E_{2k}^4 - 4V^4}} \left\{ \omega_3'' \left(\frac{1}{e^{-\beta\frac{\alpha}{2}} e^{\beta\omega_3''} + 1} - \frac{1}{e^{-\beta\frac{\alpha}{2}} e^{-\beta\omega_3''} + 1} \right) \right. \\
& \left. - \omega_4'' \left(\frac{1}{e^{-\beta\frac{\alpha}{2}} e^{\beta\omega_4''} + 1} - \frac{1}{e^{-\beta\frac{\alpha}{2}} e^{-\beta\omega_4''} + 1} \right) \right\} \quad (34)
\end{aligned}$$

Using equations (31), (32) and (26) in equation (25), we can derive the $h(T)$ as

$$h(T) = -\frac{N(o)}{2} g\mu_B \int_{-\frac{W}{2}}^{+\frac{W}{2}} d\epsilon_o(k) \left\{ - \left[F_1(\vec{k}, T) - F_2(\vec{k}, T) \right] - \left[F_3(\vec{k}, T) - F_4(\vec{k}, T) \right] \right\}$$

or

$$h(T) = \frac{N(o)}{2} g\mu_B \int_{-\frac{W}{2}}^{+\frac{W}{2}} d\epsilon_o(k) \left\{ \left[F_1(\vec{k}, T) - F_2(\vec{k}, T) \right] + \left[F_3(\vec{k}, T) - F_4(\vec{k}, T) \right] \right\} \quad (35)$$

Equations (21) and (35) are the final expressions for superconducting order parameter (Δ) and staggered anti-ferromagnetic order parameter(h). We have made all the parameters used in the above equation dimensionless by dividing them by $2t$. The band width of the conduction band is taken as $W=8t$. Thus the dimensionless parameters are redefined as

$$\frac{\Delta(T)}{2t} = z \quad \text{and} \quad \frac{h(T)}{2t} = h$$

$$\frac{\epsilon_o(k)}{2t} = x_0, \quad \frac{\alpha}{2t} = \alpha, \quad \frac{k_B T}{2t} = \theta$$

Using the dimension-less quantity like phonon frequency $\frac{\omega_D}{2t} = \tilde{\omega}_D$, the conduction bandwidth $\frac{W}{2t} = \tilde{W}$, the strength of the hybridization $\frac{V}{2(t)} = \tilde{V}$ and the coupling constants $N(0)V_0 = \lambda_1$ (i.e,superconducting coupling constant), $N(0)g\mu_B = \lambda_2$ (anti-ferromagnetic coupling constant), the equations can be rewritten as

$$z = -\lambda_1 \int_{-\tilde{\omega}_D}^{+\tilde{\omega}_D} dx_0(\mathbf{k}) [F_1(x_0, \theta) + F_2(x_0, \theta)] \quad (36)$$

and

$$h = \lambda_2 \int_{-\frac{\tilde{W}}{2}}^{\frac{\tilde{W}}{2}} dx_0 [(F_1(x_0, \theta) - F_2(x_0, \theta)) + (F_3(x_0, \theta) - F_4(x_0, \theta))] \quad (37)$$

In the above equations (Δ), h are self consistent equations. Thus in order to study these quantities with temperature, it is important to have the knowledge about the nature of the co-existing phase and these two equations have to be solved self-consistently. In our calculation the localised energy level is assumed to coincide with the Fermi level i.e. ($\epsilon_F = 0$) as determined from band structure calculation [5].

3 Results and Discussion

In our calculation, we have obtained two parameters, superconducting gap function (Δ) and the staggered anti-ferromagnetic gap function (h) as given in equation (36)

and (37), which are coupled to each other. These equations are solved numerically and self-consistently in presence of magnetic field. We have used a standard set of parameters [5,6,19], like superconducting coupling $(\lambda_1) = 0.111$, anti-ferromagnetic coupling $(\lambda_2) = 0.1598$, staggered magnetic field $(h = 0.001 \text{ to } 0.005)$, conduction band width $(\tilde{\omega}_D = 1 \text{ eV})$, temperature parameter $(\theta = 0.001 \text{ to } 0.005)$ and hybridization strength $(V = 0.002 \text{ to } 0.0015)$. In an external magnetic field, the presence of hybridization in the Hamiltonian produces extra terms $(F_3 \text{ and } F_4)$ in the equation for staggered magnetic field. Fig-1. shows the temperature dependence of superconducting and anti-ferromagnetic order parameter for different external magnetic field. Superconducting gap increases with decreasing temperature and has an almost constant value around Θ_N . In presence of external magnetic field the superconducting gap is suppressed in the pure phase due to intervene of magnetic moment of impurity preventing the formation of spin up or spin down cooper pairs referring to as pair breaking. On the other hand superconducting gap is increased in the coexisting phase in an external magnetic field. When the external magnetic field is increased steadily from 0.0002 (about 0.86T) to 0.0020 (about 8.63T), critical temperature parameter Θ_c decreases constantly from 0.0044 (equivalent to the temperature 12.69K) to $\Theta_c = 0.0042$ (about 12.12K). The calculated superconducting gap $\frac{2\Delta_0}{k_B T}$ increases from 1.46 to 1.62 agrees with the experimental results [9]. This is due to fact that when magnetic field is applied splitting of degenerate band takes place. Hence electron density of state increases which results in increasing the probable availability of electron for cooper pairing. Thus superconducting order parameter increases towards lower temperature range below T_N which agrees quite well with previous result [18]. From the graph it is observed that in presence of external magnetic field, Neel temperature get reduced from 5.74K to 4.14K whereas antiferromagnetic gap parameter $\frac{2\Delta_0}{k_B T_N}$ decreases from 4.49 to 4.14. Neel temperature around 5K, shows good agreement with our earlier calculation and experimental result [19,22].

In figure-2. we have shown the effect of hybridization on superconducting and AFM order parameter. Both the order parameters get reduced with increase in hybridization. The hybridization plays an important role on z and h . In presence of hybridization of localized level with conduction band, the density of state at Fermi level is reduced thereby reducing T_c and T_N . The value of $\frac{2\Delta_0}{k_B T_c}$ increases from 1.46 to 1.62 and that of $\frac{2\Delta_0}{k_B T_N}$ increases from 3.49 to 4.04 with increasing V . Since the localized level lie at the Fermi level electrons from localized level can be transferred into Fermi level due to thermal fluctuation. This contribute to cooper pairing in case of superconducting state and Neel ordering in case of anti ferromagnetic state. However, towards lower temperature range below Neel temperature, superconducting order parameter remains unaffected when hybridization is increased. The critical

temperature and Neel temperature decreases with increase of V . Here we have observed that the effect of hybridization is more drastic on the Neel ordering parameter as compared to superconducting order parameter in presence of external magnetic field.

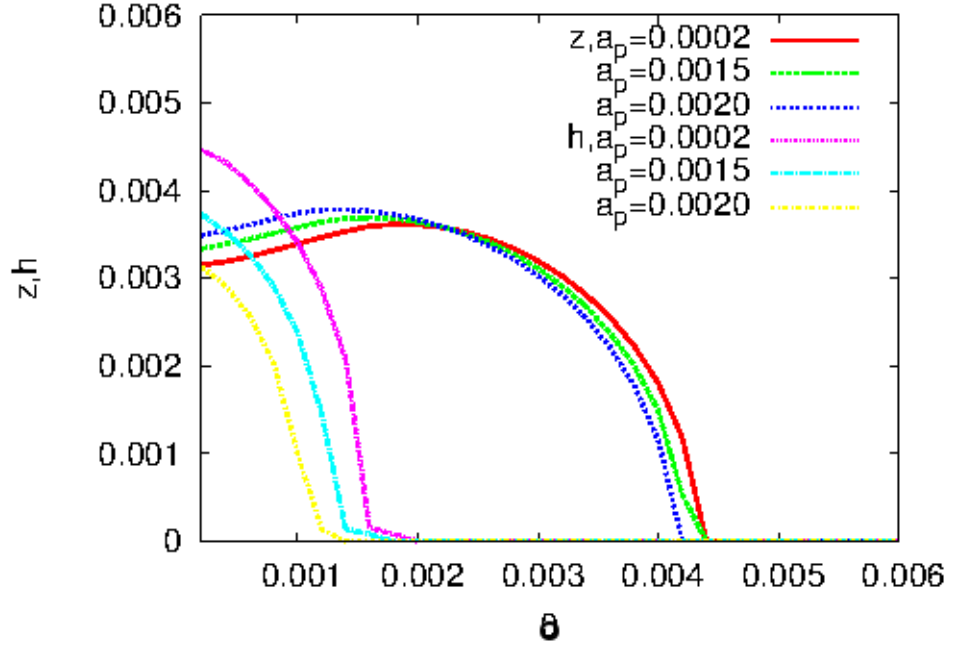


Figure 1: Sc gap(z) and AFM gap (h) vs. temperature for $v=0.002$ and various magnetic field. The superconducting coupling $\Lambda = 0.111$, AFM coupling constant $\Lambda_1 = 0.1598$, $w_D = 0.19$

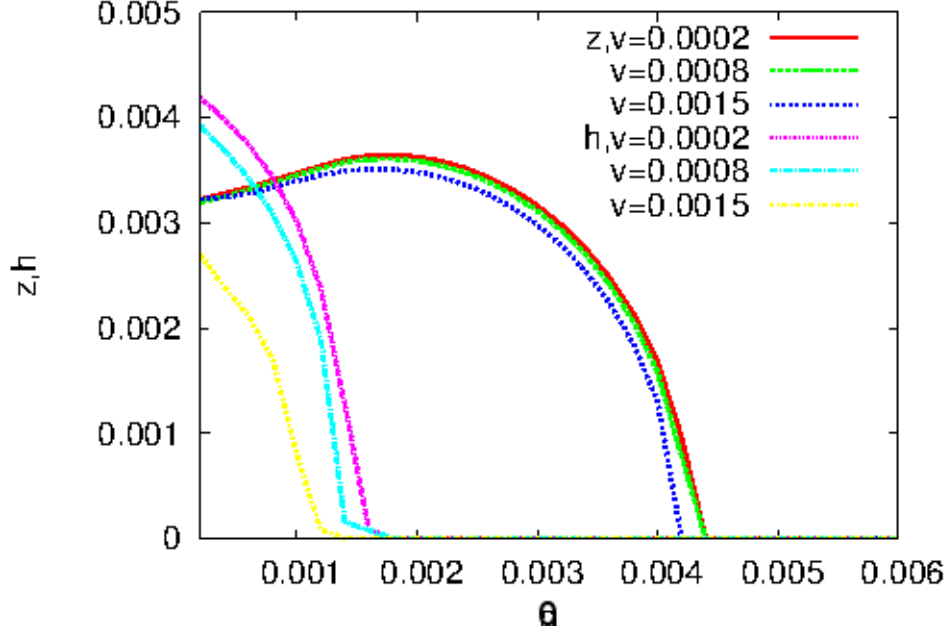


Figure 2: Superconducting gap (z) and AFM (h) at 2 Tesla magnetic field for various hybridization parameter

4 Conclusion

In this paper we have extended the model proposed by Panda et al [19] to take into account the effect of external field contribution in presence of hybridization. Along with other contributions, we have incorporated magnetic field contribution in the model Hamiltonian [17,18,19] and obtained the expression for order parameters. We have derived single particle Green's function using Zubarev's technique [21] and solved the superconducting and antiferromagnetic order parameters self-consistently with Fermi level at the middle of the conduction band. The variation of superconducting and anti-ferromagnetic order parameter for different magnetic field is studied. The results are shown graphically which indicate similar trends as that of experimental result[22]. It is observed that hybridization reduces the long range magnetic order as well as Neel temperature but superconducting gap parameter remain unaffected in the co-existing phase below T_N . We have presented a simple model, which can account for the effect of external magnetic field on the co-existing states of superconducting and anti-ferromagnetism of Yttrium Nickel boro carbide in presence of hybridization. Similar studies for other compounds is being carried

out.

Acknowledgments

The authors gratefully acknowledge the useful discussions and technical input received from Dr. Prafulla Kumar Panda, Reader in Physics, Utkal University, Odisha, Prof.R.N.Sahu, Prof.G.S.Tripathi, Berhampur University and Sri Santosh Kumar Sahu, Brahma Nagar-2nd Lane, Berhampur. The authors also would like to acknowledge all those who have helped directly or indirectly for completion of this work. The co-author Mr.P.Ch.Padhi passed away in the final stage of this work. My special acknowledgment for his dedication, endeavor and commitment in initiating this piece of research and for his valuable suggestions to give it a final shape.

References

1. P. C. Canfield, P. L. Gammel and D.J. Bishop, Phys.Today **51** (10),40 (1998).
2. R. Nagarajan, C. Mazumadar, Z. Hossian, S. K. Dhar et.al. Phys.Rev.Lett.**72**,274 (1994).
3. Rare earth Transition Metal Borocarbides, superconductivity, Magnetic and Normal state prproperties, edited by K.H.Muller and V.Naozhnyi (Kluwer Academic, Dordrecht, 2001) Rep.Prog. Phys.**64**,943 (2001).
4. A. Amici, P. Thalmeier and P. Fulde, Phys.Rev.Lett **64**, 943 (2001).
5. W. E. Picket and D. J. Singh Phys.Rev.Lett **72**, 3702 (1994)
6. L. F. Mattheiss Phys.RevB**49**, 13279 (1994).
7. K. D. D. Rathnayaka, A. K. Bhatnagar, A. Parasiris, D. G. Naugle, P. C. Canfield and B. K. Cho Phys.Rev.B**55**,8506(1997).
8. K.Maki, P.Thalmeier and H.Won, Phys.Rev.B **65**, 140502 (2002);
9. I. K. Yanson, V. F. Fisun, A. G. M. Jansen, P. Wyder, P. C. Canfield, B. K. Cho, C. V. Tomy and D. M. Paul Low.Temp.Phys **23**,712(1997).
10. C. C. Thellwarth, P. Wavins and R. N. Shellon Phys.Rev.B **53**,2579(1996).
11. V. Metlushko et.al. Phys.Rev.Lett. **79**,1738 (1997).
12. K. Izawa et.al.Phys.Rev.Lett**89**, 137006 (2002).
13. K. Izawa et.al. Phys.Rev.Lett **86**,1327 (2001).
14. S. A. Carter et.al. Phys.Rev.B**50**, 4216 (1994).
15. T. Yokoya et.al. Phys.Rev.Lett.**85**, 4952 (2000).
16. R. Coehoorn Physica C**228**, 331 (1994).
17. P. Fulde, V. Zenui, G. Zuricknagl Z.Phys B**92**, 133 (1993); P. Fulde, J Low Temp Phys **95**, 45 (1994).
18. S. N. Behera, B. N. Panda, G. C. Rout, P. Entel International Journal of Modern Physics B**15**, 2519 (2001); B. K. Sahu and B. N. Panda Modern Physics Letter B**24**, 2879 (2010).

19. B. K. Sahu and B. N. Panda *Pramana* **77**, 4, 715 (2011); B. K. Sahu and B. N. Panda *Physica C* 51335 (2015).
20. G. C. Rout, B. N. Panda and S. N. Behera *Physics C***333**, 104 (2000).
21. D. N. Zubarev *Sov Phys Usp* **95**, 7 (1960).
22. D. L. Bashlakov et.al. *Journal of Low temperature Physics***147** 314, 335 (2007).